UNCERTAINTY QUANTIFICATION IN COMPUTATIONAL STRUCTURAL DYNAMICS: A NEW PARADIGM FOR MODEL VALIDATION

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ABSTRACT. We present an overview of new research efforts underway at Sandia National Laboratories to understand the sources of uncertainty and error in computational structural dynamics and other physics simulations, and to quantify their effects on predictive accuracy. In order to establish confidence in computational simulations as these simulations move further from the established experimental database, a new approach to modeling and simulation validation is needed. In particular, when simulations are used to qualify the safety and reliability of systems, we believe that validation should be based upon a comprehensive quantification of uncertainties and errors from all phases of the modeling and simulation process. Uncertainty and error quantification is a two-step process, the first step being the identification of all uncertainty and error sources in each phase of modeling and simulation. The second step is the assessment and propagation of the most significant uncertainties and errors through the phases of the modeling and simulation process to the predicted response quantities. This paper outlines the phases of modeling and simulation, the distinction between uncertainty and error, and a categorization of uncertainty and error sources in each phase of modeling and simulation. We also address the question of how uncertainties in the form or structure of the model might be assessed using multiple models. Examples from linear structural dynamics are given to illustrate these concepts.

1. Introduction

Model validation in structural dynamics is a well established discipline which bridges analysis and experiment. This field has traditionally focused on reconciliation of test-to-analysis results with the goal of improving the predictive accuracy of computational model-based analysis. Model validation and "virtual testing" have played key roles in the engineering development of advanced aerospace and flight systems. This is because some qualification tests simply cannot be performed (or it is absurd to do so); i.e. we don't launch a satellite to see whether it will survive launch. Other tests can be performed but are not because a completely test-based approach would be prohibitively expensive. Therefore, to some extent, nearly all advanced engineering systems rely on computational simulations to not only improve designs but also to qualify, i. e. ensure the satisfactory performance of, the system hardware and design. For this reason, validation of the computational simulations is key to ensuring the performance, safety and reliability of these systems.

In structural dynamics, the criteria typically set for validation of analysis by experiment have been geared towards deterministic analysis. These validation criteria, such as the correlation of numerical model predictions to the frequencies and mode shapes estimated from modal testing, are both qualitative and subjective. The error threshold levels are intrinsically tied to what types of qualification testing will be performed, the degree of extrapolation in the critical analyses, and the notion of a factor of safety on all safety margin stress calculations. This is not to discount the value of these thresholds: they have evolved over time and express a considerable degree of expert knowledge and experience. For any particular modeling and simulation analysis, however, this type of validation does not enhance our understanding of the predictive accuracy of the analysis as we use the model to extrapolate from our measured database.

Some researchers in computational structural dynamics have used statistical techniques in parameter estimation to begin to address uncertainties [1], and have also considered the use of both uncertain parameters and historical test-analysis correlation measures to determine predictive accuracy intervals for linear and nonlinear structural dynamics modeling and simulation [2]. The primary motivations for

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addressing uncertainties are a.) the stochastic or uncertain nature of key elements in engineering design and reliability problems, and b.) the need to establish the credibility of computational simulations.

A convergence of trends are pushing the current "way of doing things" and lead us to reconsider how computational simulation is to be used in system qualification in the future, and how those analyses are to be validated. "Smaller, cheaper, faster" implies less testing on systems which are less easily analyzed than in the past. Computational technology provides tools for improving analysis predictions by reducing discretization errors and reducing the degree of analysis simplification by enabling more detail and better handling of coupled multiphysics. Unfortunately, systematic improvements in analysis predictions have not been seen as computational technologies have improved. We believe a key reason is that total errors are being driven more by modeling simplification than by solution errors. It is also possible that significant discretization and solution errors are still present, but that they are not being detected because of a lack of attention to mesh convergence issues. Finally, it may be that increased grid resolution has simply replaced modeling and solution errors at the macro scale with lack of knowledge (e.g. unknown joint physics) at the micro level.

In order to establish confidence in computational simulations as these simulations move further from the established experimental database, a new approach to modeling and simulation validation is needed. In particular, when simulations are used to qualify the safety and reliability of systems, we believe that validation should be based upon a comprehensive quantification of uncertainties and errors from all phases of the modeling and simulation process. This quantification would consider uncertainties arising from both continuous parametric uncertainties, such as variability in a geometric dimension or material property, and discrete modeling uncertainties, such as uncertainty about the physics equations governing joint compliance. In addition, quantification of errors would include numerical solution errors, such as those arising from grid resolution, as well as modeling errors, such as simplified modeling assumptions.

We believe there are two stages to uncertainty quantification: first, identification of all error and uncertainty sources; and second. assessment and propagation of uncertainty and error effects through the simulation to output quantities. This paper will present a general classification of all sources of uncertainty and error necessary to determine global estimates of uncertainty for predicted quantities of interest. This framework will then be applied to a structural dynamics problem: the prediction of peak acceleration on a circular plate due to random force excitation. Also, the sensitivity of the predicted quantity to some significant and nontraditional uncertainty and error sources, such as the partial differential equations and spatial discretization, will be examined via multiple numerical simulations.

2. Sources of Uncertainty and Error in Computational Mechanics Simulations

In this section we discuss the sources of uncertainty and error in computational simulations and propose an overall framework which categorizes these sources and their interactions. This framework is presented in greater detail in [3]. We begin by developing a new structure of the general phases of modeling and simulation. This new view is built upon combining modeling and simulation phases recognized in the disciplines of operations research and the numerical solution of partial differential equations. Within this structure, we believe that a clear distinction should be made between uncertainty and error and we propose comprehensive definitions for these terms. Specific classes of uncertainty and error sources are then defined that can occur in each phase of modeling and simulation.

2.1 Phases of Modeling and Simulation

We will use the definition of *model* given by Neelamkavil [4]: "A model is a simplified representation of a system (or process or theory) intended to enhance our ability to understand, predict, and possibly control the behavior of the system." By *modeling* we mean the construction or improvement of a model. We also use Neelamkavil's definition of *simulation*: "A simulation is the process of imitating (appearance, effect) important aspects of the behavior of the system." In other words, simulation is the exercise of the model. Here we are specifically interested in the exercise of computer models, i.e., computer codes based on mathematical models.

After reviewing existing literature in both the operations research and computational mechanics fields, we have developed a representation of the phases of modeling and simulation appropriate to systems or processes analyzed by the numerical solution of partial differential equations (PDE's) as shown in Figure 1. These phases are preceded by an initial phase which includes the definition of the physical system and specification of the requirements or objectives of the modeling and simulation. Following this initial phase are six distinct phases which are described as follows.

<u>Conceptual Modeling</u> The conceptual modeling phase determines what physical events, or sequence of events, will be considered and what types of coupling of different physical processes will be considered. During this phase, no mathematical equations are written, but the fundamental assumptions of the events and physics are made. Only conceptual issues are considered, with an emphasis on determining all possible factors that could affect the requirements set for the modeling and simulation. It is important in this phase that all possible physics-couplings are listed that may influence the results even of they may not be considered later on in the analysis. This is critical because if events or couplings are not considered in this phase, they cannot be resurrected later in the process. This is similar to the fault-tree structure in probabilistic risk assessment of high consequence systems, such as in nuclear reactor safety analyses. Even if a certain sequence of events is considered extremely remote, it should still be considered as a possible event sequence in the fault-tree. Whether the event sequence will eventually be analyzed is not a factor in including it in the conceptual modeling phase.

<u>Mathematical Modeling</u> During the mathematical modeling phase, the precise mathematical, i.e., analytical, statement of the problem, or series of event-tree-driven problems, to be solved is developed. Any complex mathematical model of the problem, or physical system, is likely to be composed of many submodels. The complexity of the models depends on the physical complexity of each phenomenon being considered, the number of physical phenomena considered, and the level of coupling of different types of physics. The mathematical model formulated in this phase is considered to be the complete specification of all of the PDE's for all components of the system. Along with the PDE statement of the mathematical model,

all of the appropriate initial and boundary values, and the required auxiliary models must be specified for the physics considered.

Discretization of the Model The next phase is the conversion of the PDE form of the mathematical model into a discrete numerical, model. This phase takes into account the conversion of the mathematics from a calculus problem to an arithmetic problem. In the discretization phase, all of the spatial and temporal differencing methods, discretization of the boundary conditions, discretization of the geometric boundaries, and grid generation methods are specified in analytical form. In other words, algorithms and methods are prescribed in mathematically discrete form, but the spatial and temporal step sizes are not specified. This step focuses on the conversion from continuum mechanics to discrete mathematics, not on numerical solution issues. We believe that the continuum model and the discrete model should be separately represented in the phases of modeling and simulation. This phase deals with questions such as consistency of the discrete equations with the PDE's, and conversion of mathematical singularities in the continuum into discrete representations.

Programming of the Discrete Model The next phase, which is common to all computer modeling and simulation, is the computer programming phase. This phase converts the algorithms and solution procedures defined in the previous phase into a computer program. This phase has probably achieved the highest level of maturity because of many years of programming development and software quality assurance efforts. These efforts have made a significant impact in areas such as commercial graphics, mathematics, and accounting software, telephone circuit switching software, and flight control systems. Little impact, however, has been made in corporate and university developed software developed for research applications in computational mechanics.

Numerical Solution of the Programmed Discrete Model The next phase, individual numerical solutions are obtained. This phase is the most specific of all phases of modeling and simulation. At the conclusion of this phase there are no quantities left arithmetically undefined or continuous. For example, grid spacing is specified, parameters such as material constants and damping coefficients are specified, and time and space exist only at points. If uncertainty in some inputs or physical parameters of the numerical model are passed through to the numerical solution phase, as is commonly the case in nondeterministic analysis, then multiple computational solutions would be required. Consider, for example, a shock response analysis where the material elastic modulus is specified by some probability distribution. Then thousands of Monte Carlo solutions may be required to address the problem definition.

Interpretation of Results The final phase concerns the interpretation of computational results. This phase involves determining the methods for presentation of computed results into a usable form. This phase can also be described as the construction of continuous functions based on the discrete solutions obtained in the previous phase. Here the continuum mathematics formulated in the mathematical modeling phase is approximately reconstructed. This phase is specifically called out because of the sophistication of the software that is being developed to comprehend modern computational simulations. This area includes graphical visualization of results, animation, and perhaps use of sound or virtual reality. Some may argue that this phase is simply "post-processing" of the computational data. This description does not do justice, however, to the rapidly growing importance of this area and its capability for introducing unique forms of errors.

2.2 Sources of Uncertainty and Error

We now discuss the sources of uncertainties and errors that are associated with each phase of modeling and simulation, as illustrated in Figure 2. Essentially all of the individual sources of uncertainty and error described below have been pointed out by researchers in the past. Some, like computer round-off, are very well understood, even to the point that most computational analysts do not make note of it. Others are poorly understood or characterized, and it may be unclear whether they should be treated as an uncertainty or an error. For this we must first develop comprehensive definitions for uncertainty and error that are appropriate for modeling and simulation.

Definitions of Uncertainty and Error The most developed definition or understanding of uncertainty is in regard to experimental measurements. Although this is helpful, we require definitions that apply to the much broader topic of modeling and simulation. We define *uncertainty* as a *potential* deficiency in any phase or activity of the modeling process that is due to *lack of knowledge.* The first feature which this definition stresses is "potential", meaning that the deficiency may or may not occur. In other words, there may be no deficiency, say in the prediction of some event, even though there is a lack of knowledge. Whether the deficiency occurs is most commonly represented by some type probability distribution of occurrence. The second key feature of uncertainty is that its fundamental cause is incomplete information. Since the cause of uncertainty is lack of knowledge, increasing the knowledge base can reduce uncertainty.

We define *error* as a *recognizable* deficiency in any phase or activity of modeling and simulation that is *not* due to lack of knowledge. This definition stresses the feature that the deficiency is identifiable or knowable upon examination, that is, the deficiency is not determined by lack of knowledge. By this we mean that there is an agreed-upon approach which is considered to be more accurate. If divergence from the correct or more accurate approach is pointed out, the divergence is either corrected or allowed to remain. This implies a segregation of error types: error can be either *acknowledged* or *unacknowledged*. Examples of acknowledged errors are: finite precision arithmetic in a computer; physical approximations made to simplify the modeling of a physical process; a specified level of iterative convergence of a numerical scheme; conversion of the governing PDE's into discrete equations. When the analyst introduces these acknowledged errors in the modeling or simulation process, there is typically some idea of the magnitude of the error introduced. Unacknowledged errors are blunders, or mistakes. That is, the analyst intended to do one thing in the modeling and simulation, but, for example, due to human error, did another. There are no straightforward means to estimate or bound the contribution of unacknowledged errors, although steps, such as independent checks and reviews, can reduce their frequency of occurrence.

We will now detail the sources of errors and uncertainties in four of the phases discussed previously. A discussion of error sources in the programming and results interpretation can be found in [3].

Conceptual Modeling Uncertainties The dominant deficiency in the conceptual modeling phase is uncertainty, as opposed to error. Conceptual modeling uncertainties arise in the formulation of the analysis of the event, and in the lack of knowledge of the event. Figure 2 shows the two types of uncertainties associated with conceptual modeling: scenario abstraction and lack of system knowledge. By scenario abstraction we mean the determination of all possible physical events, or event sequences, that may affect the goals of the analysis. For relatively simple systems, such as low level vibration of a thin circular plate in a vacuum, scenario abstraction can be straight forward. For complex engineering systems exposed to a variety of interacting factors, scenario abstraction is a mammoth undertaking.

The second class of uncertainty listed, lack of system knowledge, refers to uncertainties that are primarily due to limited information about the system. This class clearly affects and interacts with scenario abstraction, but here we stress lack of knowledge for a specific scenario, rather than the possible existence of the scenario. Two important examples for this class of uncertainty should be mentioned. First is the lack of knowledge of the initial state of key elements of the system. For complex engineered systems, knowledge of the factors, such as the following, becomes important: was the system correctly manufactured and assembled, how well was the system maintained, and what level of uncertainty exists for the properties of the components which are important in the analysis (such as dimensions, densities, elastic moduli, etc.). The second example is lack of knowledge of future conditions affecting the system. Examples of these are environmental conditions and human interaction with the system during the event. These are examples where it is not possible to significantly reduce lack of knowledge, and reduce the uncertainty, by improved sampling of past events.

Mathematical Modeling Uncertainties and Errors Mathematical modeling contains both uncertainties and errors. Uncertainties and errors that occur in this phase arise from three mathematical sources (Figure 2): the continuum equations for conservation equations of mass, momentum, and energy; all of the auxiliary equations which supplement the conservation equations; and all of the initial and boundary conditions required to solve the PDE’s. The primary uncertainties that occur in mathematical modeling are two fold. First is inadequate knowledge of parameters in known physics. Parameter uncertainty is by far the most commonly analyzed in uncertainty analyses. The second type of uncertainty is that due to limited, or inadequate, knowledge of the physics involved. For example, not knowing the PDE’s which govern friction in a mechanical joint. Errors in the mathematical modeling phase can be equally significant. The primary errors are those due to mathematically representing the physics in a more simplified form than is known to be appropriate for the results required from the modeling and simulation. The mathematical modeling uncertainties and errors together are sometimes referred to “model form errors” or model structural errors”.

A primary example of uncertainty that occurs in the conservation equations for structural dynamics is the localized nonlinear physics of friction, contact, and impact in bolted joints. Auxiliary physical equations in the mathematical model are equations such as the material constitutive models and failure models. Examples of uncertainties in initial and boundary conditions are: inaccurately known initial velocity of a body, and imprecisely known geometry of materials because of manufacturing and assembly variances. Errors in mathematical modeling can also exist. Some examples of acknowledged errors are: assumption that a plate can be modeled using thin shell theory when three dimensional effects are important, assumption of a constant beam cross-section when the section is actually not constant, and assumption of material and geometric linearity when stresses and displacements are not small. All of these examples are of the character that physical modeling approximations were made to simplify the mathematical model and the subsequent solution.

Discretization Errors The discretization phase converts the continuum model of the physics into a discrete mathematics problem. Since this is fundamentally a mathematics approximations topic, errors and not uncertainties are the dominant issue in this phase. Some may question why this conversion process should be separated from the solution process, where the characteristic mesh size and time integration step sizes are set. We argue that this conversion process is the root cause of more difficulties in the numerical solution of PDE’s than is generally realized. This is particularly true in cases of nonlinear phenomena such as fracture dynamics and frictional contact in mechanical joints. It can also be evident in linear structural mechanics and dynamics, where the presence of singularities in the continuum model creates solution error which does to disappear as the grid size approaches zero. It is becoming increasing clear that the mathematical features of strongly nonlinear and chaotic systems can be fundamentally different between the continuous and discrete form, regardless of grid size [5,6].

As shown in Figure 2, we identify three sources of discretization error; discretization of the conservation laws, the boundary conditions, and the initial conditions. The types of errors we are pointing out here are typically very difficult to isolate. In finite differencing, one method of identifying these type errors is to analytically prove whether the method is consistent; that is, do the finite difference equations approach the continuum equations as the step size approaches zero. Related issues dealt with in this phase: are the conservation laws satisfied for finite grid sizes, does the numerical damping approach zero as the mesh size approaches zero, and do aliasing errors exist for zero mesh size. Discretization of PDE’s are also involved in the conversion of von Neumann and Robin’s, i. e., derivative, boundary conditions to difference conditions. We include the conversion of continuum initial conditions to discrete initial conditions, not because there are derivatives involved, but because spatial singularities may be part of the initial conditions. Some may argue that these discontinuities and boundary singularities do not actually occur in nature, so the issue of accuracy of representation of these is superfluous. This misses the point, however. If these features exist in the mathematical model of the physics, the issue is whether the discrete model represents them accurately; not whether they exist in nature. This is an issue of verification (solving the problem right) rather than validation (solving the right problem).

Numerical Solution Errors Numerical solution errors have been investigated longer and in more depth, than any of the errors associated with the numerical solution of PDE’s. Indeed, they have been investigated since the beginning of numerical solutions; Richardson in 1910 [7]. These deficiencies in the solution of the discrete equations are properly called errors because they are approximations to the solutions of the original PDE’s. As shown in Figure 2, we categorize these errors into four categories: spatial grid convergence, time step convergence, iterative convergence, and computer roundoff. Of these, perhaps the only one that needs explanation is iterative convergence. By this we mean the finite accuracy to which algebraic discrete equations are solved. In linear structural dynamics, iterative convergence errors can occur when iterative methods, e. g. conjugate gradients, are used to solve the large matrix equation within a time step. Iterative errors can also occur in most algorithms, such as Lanczos, used to iteratively solve the generalized symmetric eigenvalue problem. In fact, since large matrix algebra problems are typically posed at each iteration of an iterative eigenvalue method, we can encounter both inner and outer loop iterative convergence errors if iterative methods are used to solve the matrix equation. The use of iterative techniques becomes even more necessary as nonlinear phenomena are introduced into the physics; in that case many levels of iterative convergence errors may be encountered.

Although we categorize four sources of solution error, it should be noted that they are of two types. The first is due to the finite discretized solution of the PDE's; spatial grid convergence and time step size convergence are of this type. The second type is due to the approximate solution of the discrete equations, that is, what errors are made in the solution of the resulting discrete equations. Iterative convergence and round-off error are of this type and they account for the difference between the exact solution of the discrete equations and the computer solution obtained.

3. Assessment and Propagation of Model Uncertainty

In the previous section, we presented an overall framework for the phases of modeling and simulation, and within that framework categorized sources of uncertainties and errors which are important in modeling and simulation. Understanding the sources of uncertainty or error in a particular analysis problem, however, is only the first step in quantifying the total combined uncertainty and error in the simulation. The second step is to propagate those uncertainties and errors from their origin and through the subsequent phases of the simulation to determine their impact on the output of the simulation. While a great deal of attention has been given to ways of estimating probability distributions of simulation outputs given the distributions of continuous, nondeterministic inputs, relatively little attention has been paid to the model itself. By the form of the model we mean those attributes, such as simplifying assumptions, choice of PDE's, computational mesh topology, and other non-parameterized features which determine the form of the PDE's and ultimately the order of the algebraic problem. We believe that, in order to quantify the major sources of uncertainty and error in modeling and simulation, we must develop procedures to quantify the effects of these modeling errors and uncertainties.

One approach to the assessment of mathematical model uncertainty, as distinct from parameter uncertainty, is suggested by Draper [8]. This approach has been termed by Draper and others [9] as Bayesian Model Averaging, because the approach uses the Bayesian concept of prior probability densities which are then revised to incorporate new data. In statistical parameter estimation, Bayesian methods are similar to maximum likelihood estimates in that they consider the relative uncertainty or reliability of the relevant data. They are different, however, in that they also consider prior beliefs or qualitative information on the parameter being estimated, which serve to regularize the estimation.

While probability concepts are appropriate for addressing uncertainties, it is not yet clear how useful they may be in assessing the effects of modeling errors, such as acknowledged simplifying assumptions and numerical errors caused by finite spatial discretization. As discussed in the preceding section, uncertainties and errors are not equivalent. They are, however, similar in that we are interested in the sensitivity of the simulation output to both. In the present discussion and subsequent example, we will deal with multiple competing models which differ in their simplifying assumptions, element topology, and model size. While these model attributes are a combination of errors and uncertainties, we intend to apply the Bayesian model averaging approach in order to both illustrate the methodology and to begin assessing the effects of these errors and uncertainties on the simulation output.

In the problem of assessing mathematical modeling uncertainty, we must address aspects of the model which are not parameterized, at least not in continuous terms. Draper proposes that, analogous to a continuous expansion of models in a space measured by a vector of continuous parameters, we instead consider a discrete expansion of possible model structures. It is then required that the probabilities of all the models considered together sum to unity. We know that we necessarily cannot consider the potential infinity of model structures which could potentially be applied, correctly or incorrectly, to a given problem. Therefore, we seek models which are supported by expert knowledge, are supported by available diagnostic experimentation, and differ markedly in their predictions. This is because, if a model has no prior support of expert opinion, it cannot gain any support from new data. That is, the model's probability will always be zero. Similarly, if a particular model has some prior support, but no support from new data, it will eventually lose influence in competition with other models that correlate better with the data. Finally, if a number of models with nontrivial probabilities all predict the problem in the same way, they are not really contributing to the quantified uncertainty, although their relative structural diversity would enhance confidence in the uncertainty quantification itself by their representation of a large model space.

After selection of the models to be considered in such an analysis, we must then assign probabilities based on our relative beliefs in the different competing models. These probabilities might be purely subjective and qualitative, or they may begin with assumed subjective probabilities which are then updated quantitatively using relevant existing data. Then we determine prediction statistics for each model and use this information to determine prediction statistics for the space of models. That is, if y is a response quantity of interest given system input x, with a finite set $S = \{S_1, \dots, S_m\}$ of structural model alternatives, we have

$$\begin{aligned} p(y|x, S) &= \sum_{i=1}^{m} \int p(y|x, S_i, \theta_i) p(S_i, \theta_i\ |x) d\theta_i \\ &= \sum_{i=1}^{m} p(S_i\ |x) p(y|x, S_i) \end{aligned} \tag{1}$$

where θ_i are parameters of model i. This result consists of two key quantities: $p(y|x, S_i)$ is the probability density function for the response given the known data from a particular single model S_i; $p(S_i\ |x)$ is the probability of that model given the data. The result obtained is that the expected value for a response quantity of interest is weighted average of model means, and the variance is a weighted average of individual model variances plus the variance in the means of the models across the entire model space.

The use of multiple models to determine measures of model uncertainty is strongly dependent on the relative probabilities for the competing models $p(S_i \mid x)$. These probabilities can be based on purely subjective knowledge - assigning weights based on qualitative judgments. That is,

$$p(S_i \mid x) = p(S_i) \qquad i = 1, \ldots, m \tag{2}$$

where $p(S_i)$ is based on qualitative judgements, with the constraint

$$\sum_{i=1}^{m} p(S_i) = 1 \tag{3}$$

Another approach is to use relevant historical database, i.e. compute probabilities for competing models/assumptions using known data as well as qualitative assessments. In this case, the desired probabilities are given by

$$p(S_i \mid x) = \frac{p(x|S_i)p(S_i)}{\sum_{j=1}^{m} p(x|S_j)p(S_j)} \tag{4}$$

Here again we must have some prior model probabilities $p(S_i)$ which are assumed independent of the known data x and are subject to the constraint given in Eqn. 3. Then these probabilities are updated via Eqn. 4, which accounts for how well each of the models correlate with the data.

In conclusion, we note that the predictive distribution for a particular model i is given by

$$p(y|x, S_i) = \int p(y|x, S_i, \theta_i)p(\theta_i \mid S_i, x)d\theta_i \tag{5}$$

This is what most of nondeterministic analysis methods such as Monte Carlo and Latin Hypercube sampling, fast probability integration, stochastic finite elements, and reliability techniques attempt to address. That is, they determine prediction statistics for model output given uncertainty in the parameters of the model θ_i, conditional on the data x and a particular model structural choice S_i. The present Bayesian model averaging approach extends this to a space of models S using the structural probability weights $p(S_i \mid x)$.

4. Examples

In order to illustrate the ideas presented herein, we examine two problems. The objective of the first problem is to identify the sources of uncertainty and error in the simulation of a simple structural dynamics system. In the second problem, our objective is to illustrate the concept of modeling uncertainty assessment using a structural dynamics simulation with multiple models.

4.1 Uncertainty and Error Sources: Response of a Circular Plate

Our task in this problem is to predict the peak acceleration response of a free-free thin aluminum (6061-T6 alloy) circular plate at r=R/2 to applied vertical force at the center of the plate. Our objective, as stated before, is to identify all sources of errors and uncertainties likely to be encountered in the modeling and simulation of this system to meet the requirement of the analysis. The following list, although not complete, contains what we believe to be the primary sources which will influence prediction of the peak response:

Conceptual modeling uncertainties
- condition of the plate
- unknown variability in dimensions and material properties
- uncertainty in random force statistics
- environmental and system boundary conditions

Mathematical modeling uncertainties and errors
- Use of linear methods
- choice of PDE (2D or 3D)
- validity of shell theory for 2D elements
- Extension/shear/bending coupling effects
- nonsymmetry in problem if using axisymmetric elements
- mass modeling (consistent versus lumped)
- micromechanics of applied force
- variability in dimensions and material properties
- Errors in statistical methods for estimating peak response

Discretization Errors
- element selection
- force interpolation
- damping discretization
- time discretization (modal superposition vs. time integration)
- substructure reduction effects

Programming and documentation errors
- Errors in closed-form solutions
- binary format conversions
- equivalencing errors
- uncertain code defaults
- code/memory errors
- inaccurate documentation

Numerical solution errors
- finite spatial resolution
- finite temporal discretization
- iterative tolerance for eigensolver
- stiff/compliant elements increasing round-off errors

4.2 Assessment of Model Uncertainty: Frequencies of a Bracket

The second problem is to predict the free-free frequencies of vibration of a component mounting bracket and to determine confidence bounds on the predicted frequencies due to considering multiple models. In particular, we will consider variations in the geometric features included in the model, the topology and fidelity of the spatial mesh, and the types of elements used. In order to summarize the results of the different models, we will use the Bayesian model averaging approach detailed in Section 3.

The bracket, shown in Figures 3, 4 and 5, is composed of a phenolic material, whose properties are given as:

$$E \sim N(3.425\times10^6 \text{ psi}, 1.5667\times10^9 \text{psi}^2) \qquad COV = 1.116\%$$

$$\rho = 0.0689(\text{lb}/\text{in}^3)$$

That is, the elastic modulus is defined by a normal distribution with a mean of 3.425×10^{6} psi and a variance of 1.5667×10^{9} psi^{2}. The coefficient of variation (COV), which is the standard deviation as a percentage of the mean, is 1.116 %. The density is as given without any associated variability.

The three models considered are as follows:

- Model I: This model was spatially discretized using surface elements with a paving algorithm. The surface elements were then extruded into 8-noded hexahedral solid elements. The surfaces contain all of the thru holes, but fillets were not modeled. The resulting model has 31554 degrees of freedom (DOF).
- Model II: This model was meshed from a ProEngineer solid geometry definition, which contained all holes and major fillets. The solid was meshed using 10-node tetrahedral elements. The resulting model has 50565 DOF.
- Model III: This model was defined geometrically using triparametric solid regions. No holes or fillets were included in the geometry definition. These solids were then meshed with 8-node hexahedral elements. The resulting model has 53202 DOF.

Note that these three models have different levels of simplifying assumptions in their PDE form, as well as different spatial meshes and different model orders (i.e. number of discrete solution variables). Model II is the least simplified model as compared to the design problem, but it probably contains the largest solution errors. This is because tetrahedral elements are generally known to possess much poorer accuracy than hexahedral elements for the same number of grid points. Model I is the next best mathematical model and utilizes hexahedral elements to improve mesh accuracy, but the mesh size is coarser than the other models. Model III has the most significant modeling simplifications, but is superior to the other models both in terms of grid spacing and grid regularity.

In order to integrate the results of the three models together, we chose equal weightings for the models. This reflects the mixture of subjective judgments on the relative merits of the models. In addition to the three models considered, the uncertainty in the elastic material modulus was also propagated through the analysis via linear sensitivity. The results are summarized in Figure 6. The solid line represents the mean value for the predicted modal frequencies, while the dashed lines represent the ±2 standard deviation interval due to the uncertainty in the elastic modulus. Finally, the dot-dash lines are the total ±2 standard deviation "uncertainty" interval due to both the modulus and the difference between the model predictions. Note that for some modes, there is a negligible contribution from the modeling variance, while for other modes this variance is larger than the uncertainty caused by the elastic modulus. As might be expected, the model "uncertainty" increases as the mode number increases. This type of analysis could be valuable in determining where the predictive accuracy of a set of models begins to break down.

5. Conclusions

This paper has presented a framework for the phases of modeling and simulation in structural dynamics and other computational mechanics disciplines. Using this framework, sources of uncertainties and errors have been categorized. Documenting these sources is the first step towards the goal of quantifying their effect on the accuracy of the simulation. Quantification of uncertainties and errors is, we believe, a proper context for developing new principles for code verification and model validation and for ultimately enhancing the predictive accuracy of modeling and simulation. Furthermore, this paper begins to address the problem of assessing and propagating modeling errors and uncertainties, which are significant contributors to total simulation errors. This work is closely aligned with other ongoing research in nondeterministic methods, so that ultimately a comprehensive methodology for uncertainty quantification can be developed which applies to structural dynamics, as well as other computational mechanics, heat transfer, and coupled field problems.

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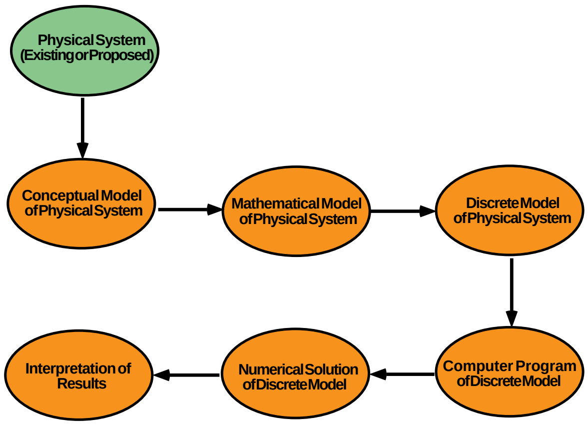

Figure 1: Proposed Phases of Modeling and Simulation

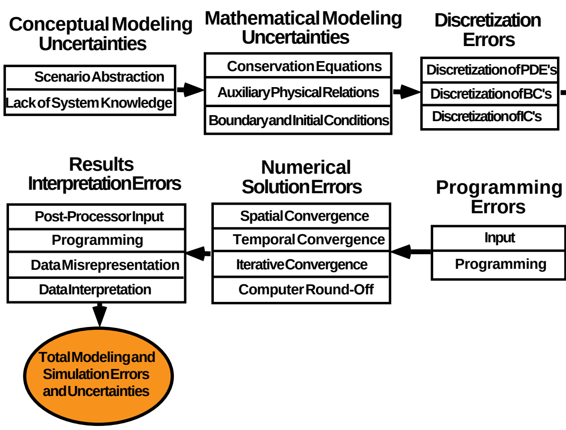

Figure 2: Sources of Uncertainty and Error in Modeling and Simulation

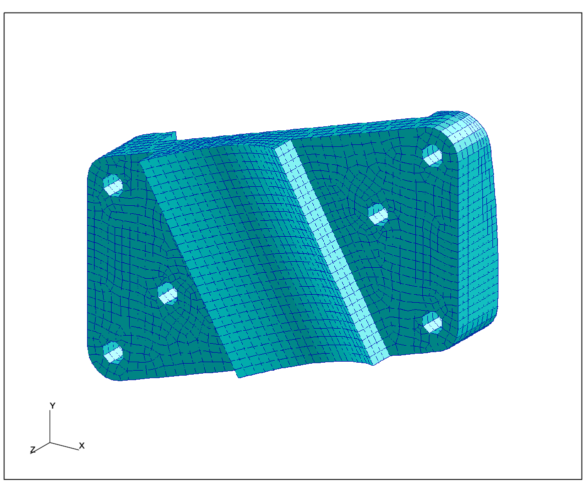

Figure 3: Model I: Paved/Extruded Hex Mesh w/hole detail (no fillets) n=31554

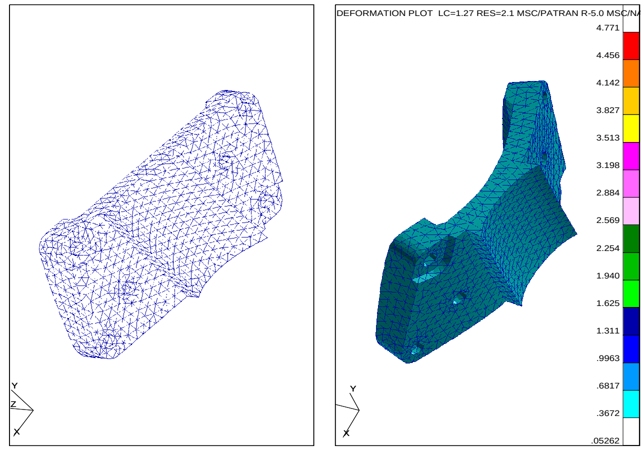

Figure 4: Model II: ProE geometry (holes and fillets) meshed w/10-node tet elements n=50565

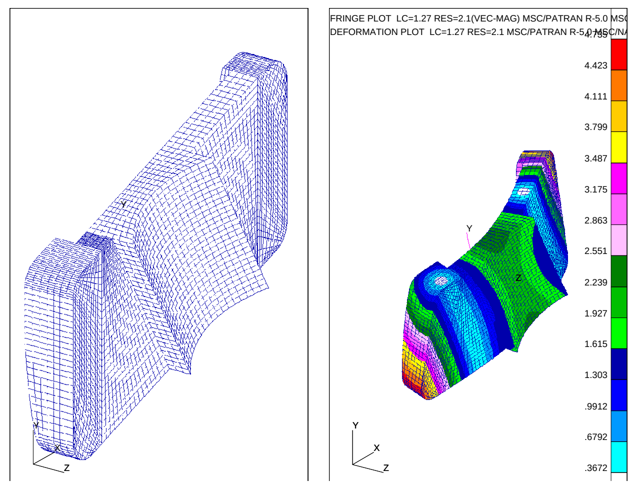

Figure 5: Model III: Triparametric Hex Mesh w/no hole or fillet details n=53202

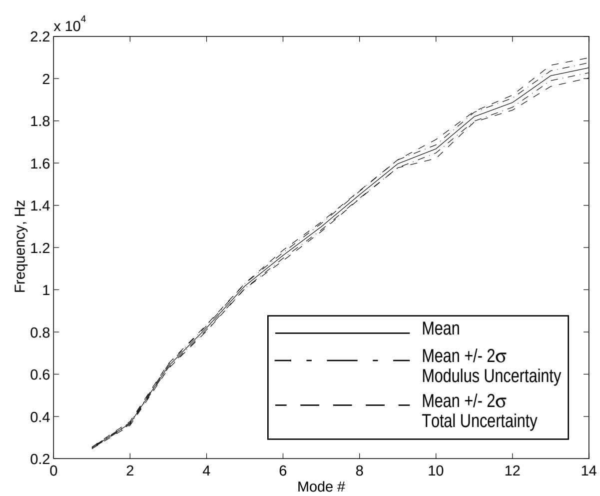

Figure 6: Uncertainty Analysis using Equal Assumed Probabilities